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Gas-Surface Interaction Model Evaluation for DSMC Applications

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Abstract. The general gas-surface interaction event is considered to be parameterized by the molecule's incident energy magnitude and incident angle relative to the surface normal. These parameters are used to estimate the degree of nonequilibrium that arises for typical applications, and the quality of scattering predictions made by common few-parameter models such as the Maxwell model. Experimental measurements and molecular dynamics simulations are evaluated as potential sources of data to develop or test improved models. An ad hoc model is used to quantify the effect that improved physical realism of nonequilibrium scattering events may have on typical surface quantities of interest for a realistic application in the rarefied regime. The model allows incremental or piecemeal incorporation of scattering data as they become available.

INTRODUCTION

Perhaps the most common gas-surface interaction (GSI) model used in Direct Simulation Monte Carlo calculations is the single-parameter Maxwell model [1], where the molecule scatters diffusely, fully accommodated to the surface temperature, with (constant) probability P_D, and scatters specularly with probability $1 - P_D$. The model can be calibrated to reproduce a macroscopic property such as surface heat flux under certain conditions, with the implicit understanding that each scattering event has essentially no physical realism. The simplicity and robustness of the model often leads to its application far beyond the range of conditions for which it has been tested or calibrated. While no method has been proposed to generalize or extend the Maxwell model, several few-parameter models are now available [2, 3] that attempt to satisfy desirable theoretical features of the scattering kernel (such as reciprocity at equilibrium) while offering some qualitative improvement to predictions relative to the simple Maxwell model.

As available computational power has increased, it has become desirable to implement more realistic (and complex) models for molecular processes into DSMC. The physical complexity of the general GSI event is such that no complete analytical model can be expected to be developed. Molecular dynamics (MD) codes are available that can deterministically predict the trajectory of a molecule as it approaches, interacts with, and scatters from a surface. Practical limitations related to addressing the wide range of expected parameters make the development of a comprehensive database from these simulations difficult. Generalization of MD techniques to consider, e.g., multi-dimensional potentials necessary to describe polyatomics [4], is still an area of active research.

As such, it appears that a GSI model that can combine desirable features typical of existing simple phenomenological models, while allowing incremental incorporation of detailed scattering data, would be useful. In the remainder of this paper we discuss the requirements of such a model for general DSMC applications, summarize recently available GSI data, formulate the model, and discuss calibration and error estimates. Finally, we present results for a sample problem to show the magnitude of the effect of differences in scattering models on surface features typically of interest in rarefied aerophysics applications.

MOTIVATION

The coordinate system used to describe the scattering process in the experimental (lab) frame of reference is shown in figure 1 (left figure). The incident state I is described by the energy e_i, angle relative to the surface normal θ_i, and azimuthal angle ϕ_i (not shown). The reflected or scattered state R (denoted by subscript r) is analogous. Implicit in

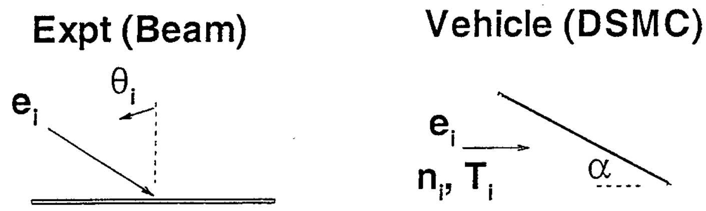

FIGURE 1. Surface interaction coordinate system and hypersonic model problem notation

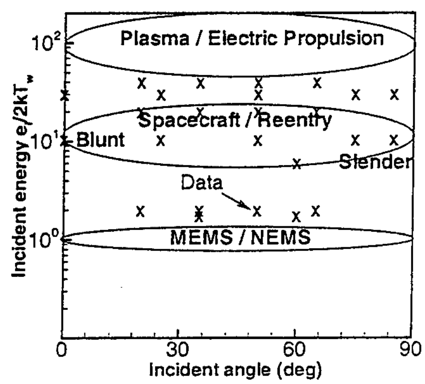

FIGURE 2. Typical magnitudes of incident properties

this description are properties of the incident gas (species, mass, etc.), and of the surface material itself (roughness, temperature, crystal orientation, etc.). In the present study, we consider a neutral monatomic gas, possessing only a translational energy component, and measure ϕ relative to the plane formed by the incident velocity vector and the surface normal.

Figure 2 gives typical magnitudes of the incident properties for several common applications. At equilibrium (stationary gas with temperature $T_g = T_w = T$, where subscript w refers to the wall) the average (i.e., flux-weighted) incident energy becomes $\langle e_i \rangle = 2kT_w$, while the average incident angle $\langle \theta_i \rangle = 45°$. Note that the normalized energy used in Figure 2 and the following is intended to indicate the degree of nonequilibrium, rather than to serve as a rigorous similarity parameter. Nonequilibrium for the present purposes refers to the magnitude of the difference between the average state of the reflected and incident fluxes, with the assumption that the relaxation from the nonequilibrium state dominates properties of interest in many complex problems to which DSMC is regularly applied.

For a MEMS device operating at room temperature and pressure, the expected deviation from equilibrium is relatively small. Ketsdever *et al* [5] perform a parametric study to assess the influence of GSI model features on the design and optimization of a MEMS propulsion system that operates near equilibrium. For a reentry vehicle or spacecraft, the large relative velocity between the body and the ambient freestream atmosphere can give rise to large nonequilibrium. The geometrical configuration (i.e., orientation) of the surface such as bluntness or slenderness can further affect the scattering properties important for, e.g., aerodynamic predictions. The presence of a shock layer ahead of the body can greatly alter incident properties from freestream values (see below). Electric propulsion applications may involve the impact of highly accelerated charged particles toward a surface at much greater than gas-dynamic energies. In the present study we focus on the moderate nonequilibrium (hypersonic vehicle or spacecraft) case.

Figure 2 also indicates several recent MD [6, 7, 8] and experimental [9, 10, 11, 12] studies of interest to DSMC GSI model development. Each is typically done at a few discrete incident energy and angle pairs. Experimental data typically include reflected speed distributions and in-plane angular intensity distributions, while MD results can provide essentially all properties of interest to DSMC.

If the incident state expected in a DSMC calculation can be determined *a priori* to be sufficiently close to the conditions used in the MD 'experiment,' the raw MD data can be used in tabulated form to provide improved representation

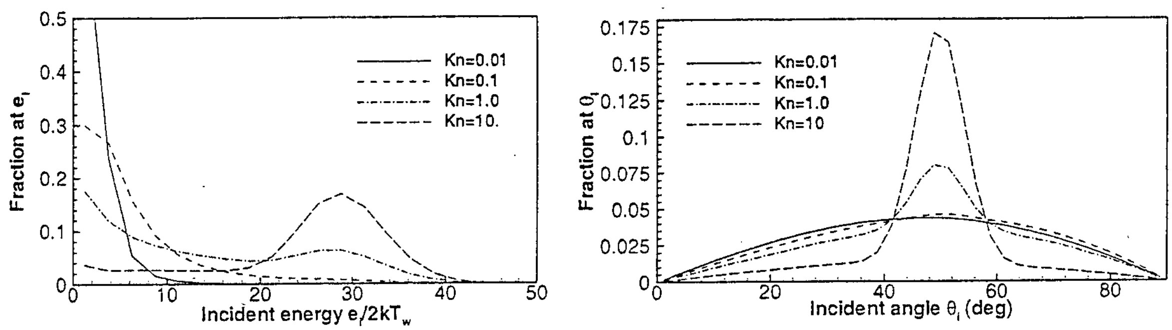

FIGURE 3. Effect on Knudsen number on incident energy distribution $f(e_i)$ and incident angle distribution $f(\theta_i)$

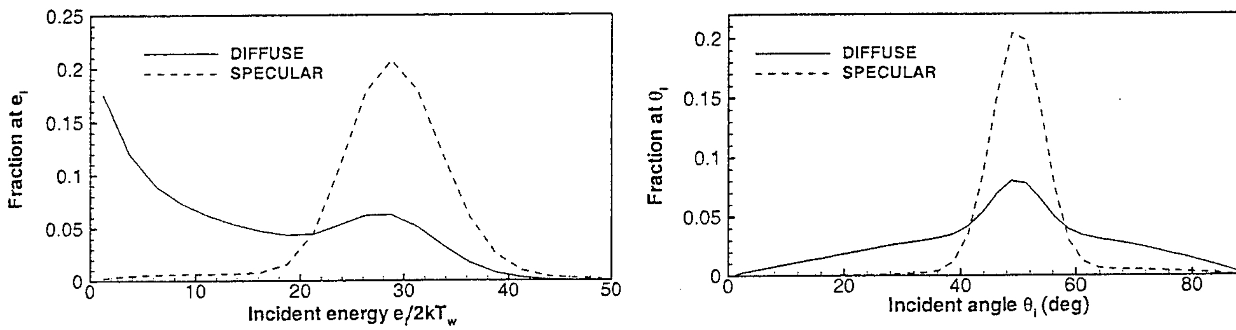

FIGURE 4. Effect on surface model on incident energy distribution $f(e_i)$ and incident angle distribution $f(\theta_i)$, Kn=1.0

of each scattering event. The robustness and generality of this type of approach are questionable, however. Extrapolation or interpolation to account for different freestream conditions is problematic. Worse, intermolecular collisions can greatly alter the incident distribution for a finite Knudsen number. To assess the dominant characteristics of the incident distribution under these conditions, DSMC calculations were performed for a model problem of a one meter flat plate at angle of attack $\alpha = 40°$ at hypersonic velocities (Figure 1, right figure). The freestream conditions and the wall temperature were chosen to correspond to the data of Cook & Hoffbauer [11] (N_2 - SiO_2, $e_i/2kT_w = 28.4, T_w = 300K$).

Figure 3 shows the directly sampled incident energy (e_i) distribution and angle (θ_i) distribution with the Knudsen number Kn (based on the freestream properties and the plate length) as a parameter. The values are averaged over the complete windward face of the plate. Clearly, intermolecular collisions in the shock layer give rise to a multi-modal incident distribution. The distribution consists roughly of an undisturbed freestream component, a component representative of molecules previously accommodated to the (cold) wall temperature, and a component representative of molecules that have undergone partial equilibration (multiple intermolecular collisions) with a broad energy range comparable to the shock layer or stagnation temperature. Note that intermolecular collisions are performed here with the VHS model, which does not accurately resolve the details of the scattering process under nonequilibrium conditions. Obviously, the shock layer and surface model are coupled for finite Kn. Figure 4 shows the effect of the surface model using the diffuse ($P_D = 1$) (as used in figure 3) and specular ($P_D = 0$) limiting cases of the Maxwell model for Kn= 1.0. Wilmoth *et al.* [13] have performed similar parametric studies for a spherical body using the diffuse model only.

Referring again to figure 2, the MD (or experimental) coverage of the incident parameter space is sparse. Several approaches have been proposed to interpolate or even extrapolate the monoenergetic, mono-angular data into a form necessary for implementation in DSMC. Collins & Knox [9, 10] develop correlations for the variation of the Nocilla model [14] parameters with incident angle based on experimental data at large incident energies. Cook & Hoffbauer [11] provide a method to extract Nocilla parameters for arbitrary energy and orientation from experimental measurements of forces. Rettner [12] has developed a model based on fitting experimental data to an assumed bimodal distribution (similar to two drifting Maxwellians). Each of these studies involves different combinations of incident gases and surface materials, thus, for a given system usable data are much more sparse than that shown in figure 2. Ultimately, since the experimental measurements typically do not provide detailed distributions of scattered quantities, validation of these fitting procedures can be problematic (see below).

MD simulations appear to have the most potential to generate the detailed scattering data required for GSI model development and calibration. Results appearing in the literature are typically generated analogous to experimental measurements, i.e., a monoenergetic beam (molecule) at a fixed incident angle. Independent trajectories are repeated as necessary to obtain an accurate representation of the scattered state.

For reasonable resolution of the reflected distribution of translational energy and angle(s), on the order of 10^3 trajectories may be necessary. Assuming that it is desirable to resolve the incident state to an accuracy of a few degrees in angle θ_i, and to a few percent of the most probable value of the energy e_i (see figure 2), a full database for this simple case may require $10^5 - 10^6$ trajectories (or the order of cpu-years) to generate. Generalizing the incident phase space to include, e.g., internal energy states, or accounting for different surface states, further complicates the issue. This type of extensive multi-parameter database would also be required to address other GSI topics, such as the degree to which reciprocity may hold under nonequilibrium conditions; MD analyses comparable to the experimental studies [15, 16] of this phenomenon are lacking.

It would thus appear to be practically useful to consider GSI modelling improvements to DSMC based on a combination of sparse MD or experimental data with robust few-parameter models currently in common use. The nature of the model would allow piecemeal incorporation of the MD data, resulting in incremental improvement in the physical modeling of the process for the general application.

MODEL REQUIREMENTS

A general, robust DSMC model must provide a scattering kernel $K(I,R)$ for any incident state I. In the present study we wish to improve the physical realism of the kernel relative to the Maxwell model over as much a portion of the incident phase space as possible. Quantitative descriptions are difficult to make, but generally, a realistic model should resolve the transformation of the scattering from approximately diffuse reflection to a directed, potentially multi-lobed or multi-modal shape as incident energy increases [7].

The most important theoretical feature desirable by a few parameter model appears to be the statement of reciprocity [15] at equilibrium,

$$\mathbf{c_R} \cdot \mathbf{n} K(-R,-I) \exp(-e_R/kT) = -\mathbf{c_I} \cdot \mathbf{n} K(I,R) \exp(-e_I/kT), \tag{1}$$

where $\mathbf{c}$ is the velocity vector, and $\mathbf{n}$ is the surface normal.

Practical DSMC applications may involve an arbitrary degree of nonequilibrium, and the extent to which this requirement may be relaxed or replaced is not clear. Models that fail to satisfy this constraint will lead to systematic departure from equilibrium. Choquet [17] has addressed these errors for the analogous case of redistribution of internal energy in intermolecular collisions, where the relaxation collision number Z is similar to the Maxwell parameter P_D. The single-parameter Maxwell model satisfies reciprocity since it is a linear combination of the diffuse and specular kernel. Neither of these kernels is physically realistic.

The empirical Nocilla model [14], a drifting Maxwellian distribution, has seen various recent applications [10, 11]. The parameters of the distribution are in general non-unique, and the model does not satisfy reciprocity. The model has been found to fit the lobular angular scattering distribution seen for certain problems, but it cannot reproduce multi-lobular distributions. Quantitative comparison of the predicted reflected distributions of other quantities of interest such as energy are much less common. Figure 5 compares the energy distribution predicted by the Nocilla model with the MD data of Bruno *et al* [6] (Xe-GaSe, $e_i/2kT_w = 5.8, \theta_i = 60°, T_w = 182\,\mathrm{K}$). The Nocilla model parameters were calculated using the method of Cook & Hoffbauer [11]. The MD results (190 trajectories) have been binned and selected error bars are included. The scatter present in the data makes definitive interpretation of the reflected distribution difficult, however, the results appear to show a typical multi-modal form, with a quasi-specular peak, a significant degree of super-elastic events, and a low degree of accommodation to the cold wall conditions. Complicating the quantitative evaluation of the Nocilla model, alternate fitting constraints will also produce altered Nocilla parameters [18]. Comparisons with several other common GSI models are shown in [6].

Unfortunately, it is difficult to predict the cases for which a complex, multi-modal scattering distribution will arise. The features seen in figure 5 suggest that a linear combination of independent Nocilla distributions may be more general and accurate. In the most simple case, this approach could reproduce a bimodal distribution composed of a

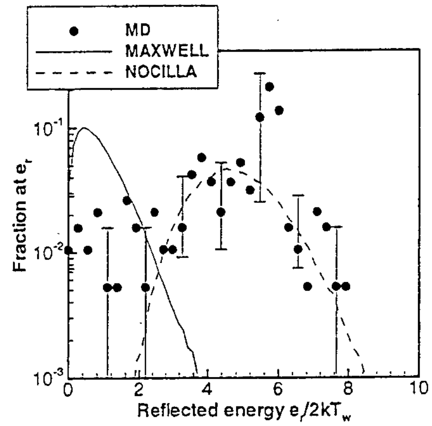

FIGURE 5. Comparison of Maxwell (Diffuse) and Nocilla models with MD [6] reflected energy distribution $f(e_r); e_i/2kT_w = 5.8, \theta_i = 60°$

"direct-inelastic" (DI, quasi-specular) component, and a "trapping-desorption" (TD, partially- or fully-accommodated) component. This type of model would have some analytical utility, if data are available for calibration (and to guide the numerical fitting procedure). Rettner [12] has fit experimental data to a TD-DI model, assuming the basic form of the reflected distributions. This model reproduces bimodal features seen in the experimental data, at the cost of several fitting parameters with limited physical justification. The complexity of these types of fitting procedures suggests that Nocilla parameterization may not be preferable over discrete (potentially voluminous) MD data in a DSMC approach where microscopic information is needed for an arbitrary incident state.

Other fitting methods have also been developed. Yamashina *et al.* [8] have used MD calculations combined with theoretical arguments to develop a Multi-Stage (MS) model. The model has been found to offer qualitative improvement over few-parameter models for some properties. The model is quite sophisticated, involving a dozen or so parameters that must be evaluated for each representative problem. The model does not satisfy reciprocity, but the magnitude of error in the uncorrected model is not clear. A heuristic was applied for use at near-equilibrium; the incident and reflected energy flux were monitored, and when the net energy flux integrated over a suitable time period was not sufficiently small the MS model was temporarily deactivated in favor of the diffuse model. This heuristic eliminates the possibility of achieving any true steady state simulation. The complexity of the model makes it difficult to estimate *a priori* the magnitude of the departure from equilibrium, and the effect it may have on properties of interest. The model below presents an alternative method to handle some of these issues.

MODEL FORMULATION

We require that the model have the capability to recover realistic features for a general nonequilibrium (i.e., high energy) scattering process. Lacking detailed data in the near-equilibrium (low energy) regime, we assume that the proposed model can reduce to common phenomenological models. Any potential relative improvement offered by this approach thus arises under highly nonequilibrium conditions, where more accurate data may predict a complex scattering pattern and thus momentum and energy exchange greatly different from (and not representable by) the simpler models.

The multi-flux (MF) model subdivides incident phase space (here (e_i, θ_i)) based on the availability of discrete detailed scattering data (or localized models) (see, e.g., figure 7, discussed below). Each subspace has a default, or background, model. For the present work, diffuse reflection is used as the default, but other models such as the CL [2] or CLL [3] models could be substituted. A foreground dataset (or model) is also defined for some or all subspaces, as available. The more accurate foreground model is applied with high probability to each impact in that subspace. The probability function is the generalized Maxwell parameter, $P_D(e_i, \theta_i)$. Here a simple form of this function is assumed to facilitate study of the basic behavior of the complete model.

We assume that the realistic nonequilibrium scattering model will not satisfy reciprocity, and thus the background model is a necessary, but not sufficient condition, to address this limitation. The degree to which reciprocity is violated

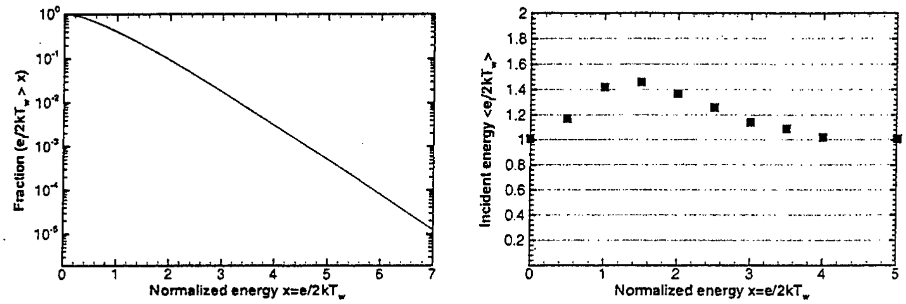

FIGURE 6. Fraction of incident molecules in an equilibrium gas with normalized energy greater than x, $F(e_i/2kT_w > x)$, (left figure), and steady state incident energy for the MF-specular model of equation (2)

is dependent on the relative flux between the subspace (which is in general dependent on the features of each model, and the probability function $P_D(e_i, \theta_i)$).

As a test case, we consider a closed one-dimensional system bounded by a wall at T_w, and a specular surface located at a distance $H/2$. The gas contained inside is initialized to an arbitrary state, and the unsteady or steady fluxes to the wall are of interest. Intermolecular collisions are not considered (i.e., Kn$\to\infty$), so that the evolution of the system is determined solely by the GSI model. The characteristic time for transport across the system $\tau = H/v_{mp}$, where v_{mp} is the most probable molecular speed at T, steady state conditions are achieved on the order of 10τ [19].

We can estimate some of the features of this approach for the simple case where specular reflection is used as the the foreground model, and the probability of a diffuse reflection is simplified as,

$$P_D(e_i) = \begin{cases} 0.2 & \text{if } e_i/2kT_w > x \\ 1.0 & \text{otherwise.} \end{cases} \tag{2}$$

The high energy value of P_D is based simply on a fit [6] of the Maxwell model to energy flux data for test conditions used below. Here, it indicates that the large majority of high energy impact events would use the 'more accurate' model. In this case, the departure from reciprocity is a function only of P_D, with steady state being achieved as a balance between the net gain and loss between the two subspaces due to diffuse reflection (the specular component makes no contribution). Variation of the foreground P_D for a given value of the energy cut-off x will show a similar effect.

Figure 6 (left figure) shows the fraction of molecules in an equilibrium gas that impact the wall with energy $e_i/2kT_w > x, F(e_i/2kT_w > x) = \Gamma(2,x)$, where $\Gamma()$ is the incomplete gamma function of [20]. The high energy tail of the energy distribution function is a negligible contributor to the number flux (but not necessarily to higher flux moments). Figure 6 (right figure) shows the steady state deviation of the incident energy from the equilibrium value as a function of the cut-off energy x for the MF-specular model with the P_D of (2). The error peaks at 50 percent, biased toward a higher average energy due to the net gain to the higher energy subspace.

RESULTS

For a given form of the foreground / background probability function $P_D(e_i, \theta_i)$, we can evaluate the relative effect of the foreground model and the degree to which the multi-flux approach may improve accuracy for different applications. Absolute assessment of accuracy is made difficult by the lack of realistic data. Various forms of the foreground function are tested: Specular with P_D as given in (2), Nocilla, or tabulated MD data; all use the diffuse background model.

We utilize the one-dimensional geometry discussed above, with the gas initialized to either a monoenergetic beam at the conditions of reference [6] ($e_i/2kT_w = 5.8, \theta_i = 60°$), or a non-isothermal case with the same average energy, i.e., $T_g/T_w = 5.8$. The MF-MD implementation utilizes the single incident trajectory dataset of [6] . The incident phase space in this case and for the MF-Nocilla form has been partitioned as shown in figure 7,

$$P_D(e_i, \theta_i) = \begin{cases} 0.2 & \text{if } e_i/2kT_w > 5, \theta_i > 45° & I_1 \\ 1.0 & \text{otherwise} & I_2. \end{cases} \tag{3}$$

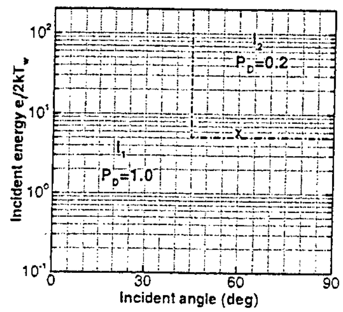

FIGURE 7. Subdivision of incident phase space for the MF case

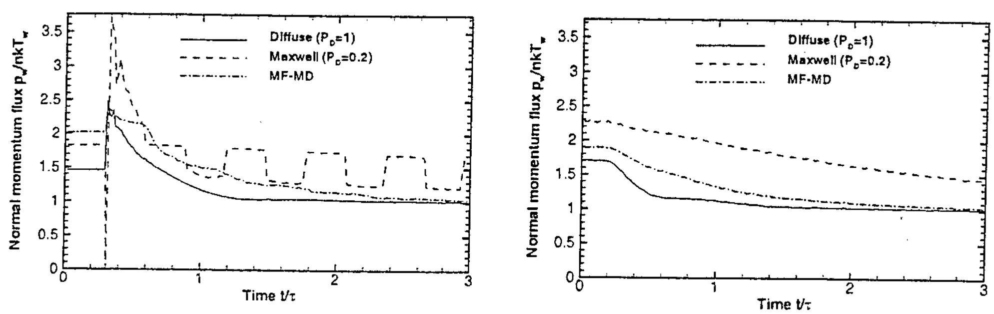

FIGURE 8. Net normal momentum flux(wall pressure) versus time for various GSI models; beam (left figure) and non-isothermal (right figure) initial conditions

At equilibrium, this partitioning results in a relative flux ratio of approximately 10^3 into the larger (I_1) and smaller (I_2) subspaces, confirming that in this case the impact of the foreground model is trivial. For the MF-MD model a random MD trajectory is selected for each accepted foreground scattering event. To maintain a more regular reflected energy state for this coarse discretization of incident space, the reflected energy is scaled as $e_r = (e_i/e_i')e_r'$, where the prime denotes values for the specific MD trajectory; the reflected angles θ_r, ϕ_r are set to the exact trajectory values.

Figure 8 shows the relaxation of the net normal momentum flux (i.e., wall pressure) for the gas initialized to monoenergetic beam conditions (left figure), and to the non-isothermal conditions (right figure). The Maxwell model shows very slow relaxation of the beam features. The MF case with the specular foreground function (not shown) exhibits similar behavior. For a purely specular wall and beam initial conditions we expect zero flux during the time periods $j\tau/[2(2e_i/2kT_w)^{1/2}\cos\theta_i], j = 1, 2, \ldots$. Though the MF-MD model contains only a single foreground function over a relatively small portion of incident phase space, instantaneous magnitudes are seen to differ from the basic diffuse model by 30 percent or more, with system relaxation time increased by a much larger factor. The MF-Nocilla case (not shown) exhibits similar behavior. Note that the MF-MD model can also adequately recover other initial reflected or net flux quantities (not shown) for the beam case, whereas the diffuse or Maxwell models can be calibrated to reproduce only one, in this case $\langle e_r - e_i \rangle$. The accuracy of the Nocilla form depends on the constraints used to fit the parameters. Comparisons of Navier-Stokes and DSMC predictions of the response of a similar system are given in [19].

CONCLUSIONS

A robust and accurate gas-surface interaction model for use in DSMC must be capable of predicting realistic scattering features for an extremely wide range of incident properties. Common phenomenological models satisfy mathematically desirable features such as reciprocity under equilibrium but lack physical realism for nonequilibrium scattering events. Much more detailed information is available from molecular dynamics simulations, however, general use of these data in a DSMC code is problematic.

An ad hoc approach that retains features of the simple models, yet allows piecemeal implementation of these more accurate data, can offer improved accuracy and reasonable robustness. Though this type of approach cannot provide insight into the details of each scattering event, it can improve realism in a DSMC context by accounting for the fact that the features of the reflected flux may be tightly coupled to details of the incident flux. Tests of a low resolution form of this model show the effect that highly nonequilibrium impact and scattering events can have on surface flux quantities typically of interest.

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